

Toluene  
108-88-3 | DTXSID7021360

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 110 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 7.22e-01

**Confidence level:** 7.43e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

1,3,5-Cycloheptatriene

**Measured:** 117

**Predicted:** 112

[Image not found](#)

Toluene

**Measured:** 111

**Predicted:** 110

[Image not found](#)

2,5-Norbornadiene

**Measured:** 89.5

**Predicted:** 99.2

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Benzene

**Measured:** 80.0

**Predicted:** 93.8